Dynamical Instabilities in a two-component Bose condensate in a 1d optical lattice

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Abstract

In this paper we carry out a stability analysis of the Bloch states of a two-component Bose-Einstein condensate confined to a 1d optical lattice. We consider two concrete systems: a mixture of two hyperfine states of Rubidium-87 and a mixture of Sodium-23 and Rubidium-87. The former is seen to exhibit similar phenomena to a single component condensate while the latter also suffers an instability to phase separation at small Bloch wave vectors. It is shown that sufficiently deep optical lattices can remove this latter instability, potentially allowing imiscible cold atoms species to be held in intimate contact and transported within an experimental system.

I. INTRODUCTION

Bloch states of weakly interacting Bose condensates have been the subject of recent experimental and theoretical study (see [1] for a review). While these states are, in many respects, similar to those of electrons in solids, they differ in one crucial respect - they are not necessarily stable [2, 3]. Isolated, weakly interacting atomic condensates are well described by mean field theory in the form of the time-dependent Gross-Pitaevskii (GP) equation. In the presence of an optical lattice this has stationary Bloch solutions of the form

$$\Psi\left(x,t\right) = e^{-i\mu t/\hbar}e^{ikx}f\left(x\right) \tag{1}$$

where $f\left(x\right)$ has the periodicity of the lattice and μ is the chemical potential for the atoms. Many of the phenomena associated with these Bloch states are familiar from the theory of electrons in solids (band structure etc.). Indeed, cold atoms systems readily exhibit phenomena which are hard to observe in electronic systems such as Bloch oscillations. However, unlike electronic states in a crystalline lattice, the Bloch solutions of the GP equation are not necessarily stable. As shown by Wu and Niu and Machholm, Pethick and Smith[2, 3], there are two types of instability. Firstly there is an energetic instability associated with Bloch states which are not local minima of the mean field energy, secondly there is a dynamical instability associated with the exponential growth of small perturbations around the Bloch state. The former instability should not be visible in systems which are perfectly described by the GP equation, which conserves the mean field energy, but will have an effect once dissipative processes become active. The dynamical instability is always significant unless the time for which the system is described by the unstable Bloch state is much shorter than the growth time for the most unstable mode.

In this paper we consider the dynamical stability of a system consisting of two distinct atomic species. The laser generating the standing wave optical lattice is supposed to have been chosen so that it is blue detuned from the nearest resonance of one species but red-detuned from the nearest resonance of the other. This means that the two species will see opposite potentials as one is attracted to the nodes of the standing wave while the other is attracted to the antinodes. We also suppose that the system is strongly confined by a cylindrically symmetric magnetic trap to ensure one dimensional behaviour.

In section 2 we review the mean field theory for such a system and the 2-component GP equation. In section 3 we consider the Bloch states of the 2-component condensate. In

section 4 we review the linear stability analysis of the mean field theory. In section 5 we consider two specific systems: firstly we consider the two species to be 2 hyperfine states of Rubidium; next we consider a mixture of Rubidium and Sodium atoms. We will see that these two examples exhibit rather different behaviour, the former is qualitatively similar to a single component system while the later exhibits quite different behaviour. In section 6 we will discuss the results obtained.

II.   MEAN FIELD THEORY FOR 2-COMPONENT SYSTEM

The mean field theory for a two component system is well described in the book by Pitaevskii and Stringari[4]. The main result is that the two component condensate wave function, $\Psi_j(x,t)$ satisfies the coupled GP equations

$$i\hbar\frac{\partial\Psi_1}{\partial t} = -\frac{\hbar^2}{2m_1}\frac{\partial^2\Psi_1}{\partial x^2} + V_1(x)\Psi_1 + g_{11}|\Psi_1|^2\Psi_1 + g_{12}|\Psi_2|^2\Psi_1 \tag{2}$$

$$i\hbar\frac{\partial\Psi_2}{\partial t} = -\frac{\hbar^2}{2m_2}\frac{\partial^2\Psi_2}{\partial x^2} + V_2(x)\Psi_2 + g_{22}|\Psi_2|^2\Psi_2 + g_{12}|\Psi_1|^2\Psi_2 \tag{3}$$

where m_j is the mass of an atom of species j and V_j is the optical lattice potential seen by species j. The nonlinear terms arise from the treatment of the atomic collisions within mean field theory. For the low temperatures relevant to ultra-cold atom experiments it is sufficient to treat the atoms as point scatterers with strengths given in terms of the relevant s-wave scattering length within the lowest Born approximation. This gives

$$g_{ii} = \gamma_{ii}\frac{4\pi\hbar^2 a_i}{m_i} \tag{4}$$

for 2-body processes in which like atoms scatter and

$$g_{12} = g_{21} = \gamma_{12}\frac{2\pi\hbar^2 a_{12}}{m_{12}} \tag{5}$$

for 2-body processes in which unlike atoms scatter. The γ_{ij}'s are form-factors accounting for the finite extent of the wavefunctions transverse to the optical lattice. For a harmonic radial trap of the form $U(r) = C^2 r^2/2$ we have

$$\gamma_{ij} = \frac{1}{\pi\left(l_i^2 + l_j^2\right)} \tag{6}$$

where the radial oscillator lengths for the two species are $l_i^2 = \hbar/C\sqrt{m_i}$. The expression for g_{12} involves the reduced mass $m_{12} = \left(m_1^{-1} + m_2^{-1}\right)^{-1}$ relevant for the "unlike" 2-body problem.

Stationary solutions of these equations of the form $\Psi_j(x,t) = e^{-i\mu_j t/\hbar}\psi_j(x)$ satisfy the time-independent GP equations

$$-\frac{\hbar^2}{2m_1}\frac{d^2\psi_1}{dx^2} + V_1(x)\psi_1 + g_1|\psi_1|^2\psi_1 + g_{12}|\psi_2|^2\psi_1 = \mu_1\psi_1 \tag{7}$$

$$-\frac{\hbar^2}{2m_2}\frac{d^2\psi_2}{dx^2} + V_2(x)\psi_2 + g_2|\psi_2|^2\psi_2 + g_{12}|\psi_1|^2\psi_2 = \mu_2\psi_2 \tag{8}$$

in which the chemical potentials of the components appear as the solution to a non-linear eigenvalue problem.

The time-independent GP equation can be obtained variationally from the mean field energy functional

$$\mathcal{E} = \int dx \left\{ \sum_j \left(\frac{\hbar^2}{2m_j}\left|\frac{d\psi_j}{dx}\right|^2 + V_j(x)|\psi_j|^2 \right) + \frac{1}{2}\sum_{ij} g_{ij}|\psi_i|^2|\psi_j|^2 \right\} \tag{9}$$

via

$$\frac{\delta}{\delta\psi_j^*(x)}\left(\mathcal{E} - \sum_j \mu_j \int dx\, |\psi_j|^2 \right) \tag{10}$$

where, as usual, the chemical potentials arise as a Lagrange multipliers enforcing the normalization conditions

$$\int dx\, |\psi_j|^2 = N_j \tag{11}$$

for a system with N_j atoms of species j.

The chemical potential of a stationary state is related to the mean field energy via the relation

$$\mathcal{E} = (\mu_1 N_1 + \mu_2 N_2) - \sum_{ij}\frac{1}{2}g_{ij}\int dx\, |\psi_i|^2|\psi_j|^2 \quad . \tag{12}$$

We consider a system in an infinite optical lattice with

$$V_j(x) = w_j\cos(\kappa x) \tag{13}$$

where $\kappa = 2\pi/d$ where $d = \lambda/2$ is the period of the lattice (half of the wavelength of the laser generating the standing wave).

III. BLOCH STATES

Next we seek Bloch states of the form

$$\phi_j^{(k)}(x) = e^{ikx}f_j(x) \tag{14}$$

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where

$$f_j(x+d) = f_j(x) \qquad . \tag{15}$$

We employ the same basic method as Machholm and Smith [3], adapted to the case of two-components. If n_j is the number of atoms of species j per unit length then the normalization condition on $f_j(x)$ becomes

$$\frac{1}{d} \int_{-d/2}^{d/2} dx \, |f_j(x)|^2 = n_j \qquad . \tag{16}$$

We also define the energy per unit length

$$E = \frac{1}{d} \int_{-d/2}^{d/2} dx \left\{ \sum_j \left(\frac{\hbar^2}{2m_j} \left| \left(\frac{d}{dx} + ik \right) f_j(x) \right|^2 + w_j \cos(\kappa x) \, |f_j(x)|^2 \right) \right. \tag{17}$$

$$\left. + \frac{1}{2} \sum_{ij} g_{ij} \, |f_i(x)|^2 \, |f_j(x)|^2 \right\} \qquad . \tag{18}$$

The periodicity of $f_j(x)$ allows us to write

$$f_j(x) = \sum_s f_{j,s} e^{is\kappa x} \tag{19}$$

so that

$$\sum_s |f_{j,s}|^2 = n_j \tag{20}$$

and

$$E = \sum_j \left(\frac{\hbar^2}{2m_j} \sum_s |f_{j,s}|^2 (m\kappa + k)^2 + \frac{w_j}{2} \sum_s \left(f_{j,s+1}^* + f_{j,s-1}^* \right) f_{j,s} \right) + \tag{21}$$

$$+ \frac{1}{2} \sum_{i,j} g_{ij} \sum_s \left(\sum_l f_{i,l+s}^* f_{i,l} \right) \left(\sum_l f_{j,l-s}^* f_{j,l} \right) \qquad . \tag{22}$$

As found by Machholm and Smith for the single component case, we can restrict our attention to real values of the f parameters and truncate summations over the Fourier label to values less than a cut-off S. We then minimize E as a function of the $2 \times (2S+1)$ f parameters subject to the constraint (20) to find the Bloch wave functions for each component for a grid of points in the range $-\kappa/2 < k < \kappa/2$ (i.e. within the first Brillouin zone of the optical lattice).

IV. STABILITY ANALYSIS

Given the Bloch state for a particular value of k, we can ask whether it is stable with respect to small fluctuations. We assume an initially small, generic fluctuation, so that the

condensate wave function has the form

$$\Psi_j(x,t) = e^{-i\mu_j t/\hbar}(\phi_j(x) + \delta\Psi_j(x,t)) \tag{23}$$

which we substitute into the time-dependent GP equation. Dropping terms non-linear in the fluctuations then gives

$$i\hbar\frac{\partial\delta\Psi_1}{\partial t} = \left(-\frac{\hbar^2}{2m_1}\frac{\partial^2}{\partial x^2} + V_1(x) - \mu_1 + 2g_{11}|\phi_1(x)|^2 + g_{12}|\phi_2(x)|^2\right)\delta\Psi_1 \tag{24}$$

$$+ g_{11}(\phi_1(x))^2\delta\Psi_1^* + g_{12}\phi_2^*(x)\phi_1(x)\delta\Psi_2 + g_{12}\phi_2(x)\phi_1(x)\delta\Psi_2^* \tag{25}$$

$$i\hbar\frac{\partial\delta\Psi_2}{\partial t} = \left(-\frac{\hbar^2}{2m_2}\frac{\partial^2}{\partial x^2} + V_2(x) - \mu_2 + 2g_{22}|\phi_2(x)|^2 + g_{12}|\phi_1(x)|^2\right)\delta\Psi_2 \tag{26}$$

$$+ g_{22}(\phi_2(x))^2\delta\Psi_2^* + g_{12}\phi_1^*(x)\phi_2(x)\delta\Psi_1 + g_{12}\phi_1(x)\phi_2(x)\delta\Psi_1^* \qquad. \tag{27}$$

As expected, the $\delta\Psi$'s are coupled to their complex conjugates and we must decouple them using a classical version of the Bogoliubov transformation, as developed by Pitaevskii[5]. We set

$$\delta\Psi_j(x,t) = e^{ikx}\left(e^{i(qx-\omega t)}u_j(x) + e^{-i(qx-\omega t)}v_j^*(x)\right) \tag{28}$$

where $u_j(x)$ and $v_j(x)$ all have the periodicity of the lattice. Substituting into the time dependent equation gives, after some manipulation, an eigenvalue problem for the $u(x)$ and $v(x)$ functions of the form

$$\mathcal{M}_{k,q}\begin{pmatrix} u_1(x) \\ v_1(x) \\ u_2(x) \\ v_2(x) \end{pmatrix} = \omega\begin{pmatrix} u_1(x) \\ v_1(x) \\ u_2(x) \\ v_2(x) \end{pmatrix} \tag{29}$$

where

$$\mathcal{M}_{k,q} = \begin{pmatrix} \mathcal{L}_1^+ & g_{11}(f_1(x))^2 & g_{12}f_2(x)f_1(x) & g_{12}f_2(x)f_1(x) \\ -g_{11}(f_j(x))^2 & -\mathcal{L}_1^- & -g_{12}f_2(x)f_1(x) & -g_{12}f_2(x)f_1(x) \\ g_{12}f_1(x)f_2(x) & g_{12}f_1(x)f_2(x) & \mathcal{L}_2^+ & g_{22}(f_2(x))^2 \\ -g_{12}f_1(x)f_2(x) & -g_{12}f_1(x)f_2(x) & -g_{22}(f_2(x))^2 & -\mathcal{L}_2^- \end{pmatrix} \tag{30}$$

and

$$\mathcal{L}_1^\pm = -\frac{\hbar^2}{2m_1}\left(\frac{\partial}{\partial x} + i(q\pm k)\right)^2 + V_1(x) - \mu_1 + 2g_{11}|f_1(x)|^2 + g_{12}|f_2(x)|^2 \tag{31}$$

$$\mathcal{L}_2^\pm = -\frac{\hbar^2}{2m_2}\left(\frac{\partial}{\partial x} + i(q\pm k)\right)^2 + V_2(x) - \mu_2 + 2g_{22}|f_2(x)|^2 + g_{12}|f_1(x)|^2 \qquad. \tag{32}$$

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Substitution of the truncated Fourier expansions

$$u_j(x) = \sum_{s=-\nu}^{\nu} \alpha_{j,s} e^{is\kappa x} \qquad (33)$$

$$v_j(x) = \sum_{s=-\nu}^{\nu} \beta_{j,s} e^{is\kappa x} \qquad (34)$$

allows this to be turned into an $4(2\nu+1) \times 4(2\nu+1)$ generalized matrix eigenvalue problem. The resultant eigenvalue problem is non-hermitian and hence need not, in general, have real eigenvalues. As shown in [6] the eigenvalues either come in real pairs $\pm\omega$ or in sets of four complex eigenvalues $\pm\omega' \pm i\omega''$. As usual in the Bogoliubov method these are not all independent. For real eigenvalues only modes with positive frequency need be considered. For the case of complex eigenvalues we may discard those with negative real parts. The presence of an imaginary part to the eigenvalue indicates an instability of the underlying Bloch state, since there will be a mode which, at least initially, grows exponentially in time at the rate ω''.

The eigenvalues for each q value form a set corresponding to the Bloch bands of the linearized fluctuation problem. Only the lowest two fluctuation bands exhibit non-zero imaginary parts to the eigenvalues, so we focus attention on these. We define the *instability* of the system with respect to modes with wave-vector q as

$$\theta(q) = \sup_{j=1,2} \left\{ \omega_j''(q) \right\} \qquad (35)$$

V. RESULTS OF STABILITY ANALYSIS

Here we will present results for the stability of the Bloch states of 2 systems. We will compare and contrast the two systems in the next section.

Firstly, we consider a system in which the two hyperfine states $|F=1, m_F=-1\rangle$ and $|F=2, m_F=2\rangle$ of Rubidium-87 are cooled in a magnetic trap to form a condensate. Such a two-component condensate was first prepared experimentally by Myatt et al[7]. We suppose that the atoms are confined by a strong axial magnetic trap and a longitudinal optical lattice. We further suppose that the laser is tuned between resonances of the two species such that $V_0 = w_1 = -w_2$ and we choose a typical value for the depth of the lattice $V_0 = 0.765 E_R$ where
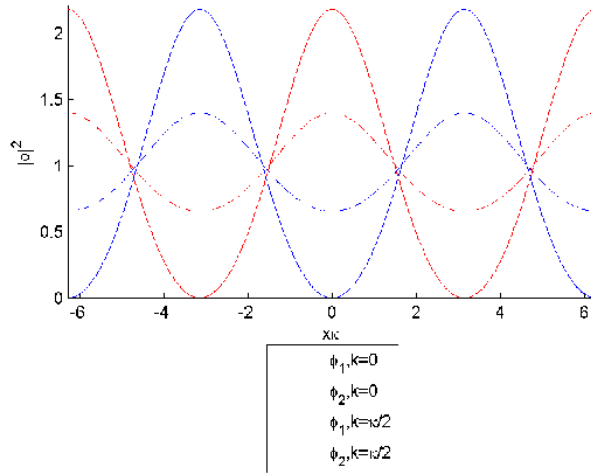
$$E_R = \frac{\hbar^2 \pi^2}{2md^2} \qquad (36)$$

FIG. 1: The Bloch wavefunctions $f_j(x)$ at $k = 0$ (dotted) and $k = \kappa/2$ (full) plotted against κx

is the recoil energy associated with a Rb atom absorbing a photon from the laser generating the standing wave. We also assume equal densities of the two species, $n_1 = n_2 = n$ and

$$ng_{11} = ng_{22} = 0.1E_R \tag{37}$$

$$ng_{12} = 0.099E_R \tag{38}$$

so that, apart from the opposite signs of the v_j's, the two species are virtually identical. In figure 1 we show the form of the Bloch functions f_1 and f_2 for both $k = 0$ and $k = \kappa/2$ (zone boundary). As can be seen, the $k = 0$ Bloch states are lightly modulated by the optical lattice with one species attracted to the nodes of the optical standing wave and the other attracted to the antinodes. The $k = \kappa/2$ Bloch states show much stronger modulation with the wavefunctions of the two species vanishing at the nodes and antinodes respectively.

Figures 2 and 3 show colour maps of the imaginary part of the fluctuation frequencies, $\omega_1''(q)$ and $\omega_2''(q)$ respectively, for the lowest two fluctuation bands as functions of the Bloch wave-vector k and the fluctuation wavevector q. As can be seen, both of the lowest bands exhibit behaviour similar to that of a single component condensate. The Bloch states are stable for $k \lesssim \kappa/4$. States with higher Bloch wave-vectors are unstable with respect to fluctuation modes with wave-vectors around $q = \kappa/2$: effectively a period doubling modulational instability. As k is increased, the unstable modes move to longer wavelengths with a greater range of q's being unstable. All of this behaviour is qualitatively similar to the behaviour of a single component condensate.
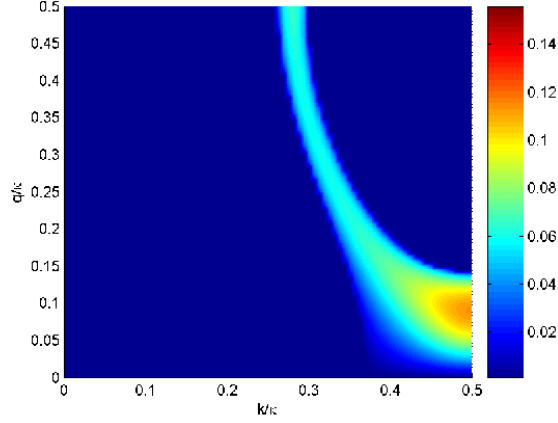
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FIG. 2: The imaginary part of the fluctuation mode frequency, $\Im\omega_1^{(k)}(q)$ for $0 < k < \kappa/2$ and $0 < q < \kappa/2$ (colour online).
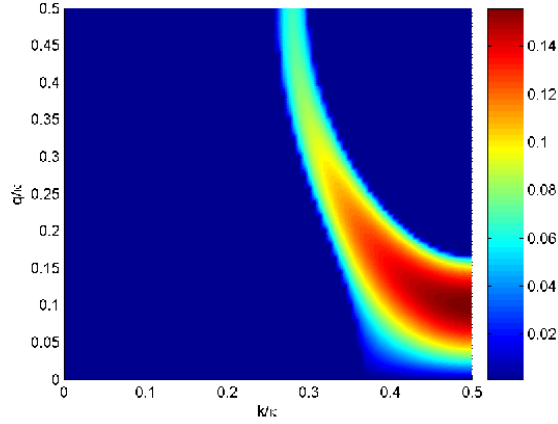

FIG. 3: The imaginary part of the fluctuation mode frequency, $\Im\omega_2^{(k)}(q)$ for $0 < k < \kappa/2$ and $0 < q < \kappa/2$ (colour online).

Now we consider a different system: a mixture of Sodium and Rubidium atoms, similarly confined to a 1d optical lattice tuned between resonances of the two species. We take typical values $V_0 = w_1 = -w_2 = 0.603E_R$ and again assume equal densities $n_1 = n_2 = n$ such that $ng_{11} = 0.047E_R$, $ng_{22} = 0.019E_R$ and $ng_{12} = 0.048E_R$. Figure 4 shows the Bloch wavefunctions for this system at $k = 0$ and $k = \kappa/2$. This system is much less symmetric and the wave functions for species 1 are more spread out due to the larger intra-species interaction. Once again the Bloch state at the zone boundary, $k = \kappa/2$, has nodes for both species. Figure 5 is a colour map showing, for each Bloch wavevector, k, and each fluctuation
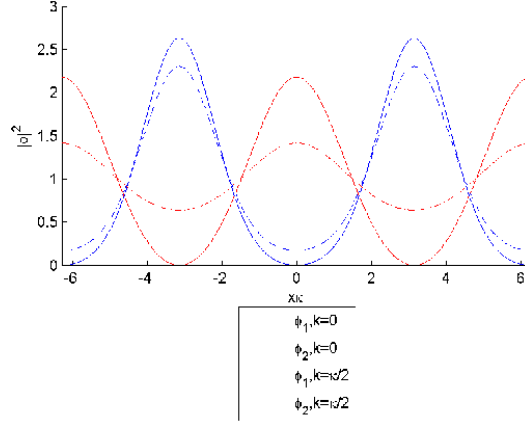
FIG. 4: The Bloch wavefunctions $f_1(x)$ and $f_2(x)$ for a Rb-Na mixture for $k = 0$ (dotted) and $k = \kappa/2$ (full).
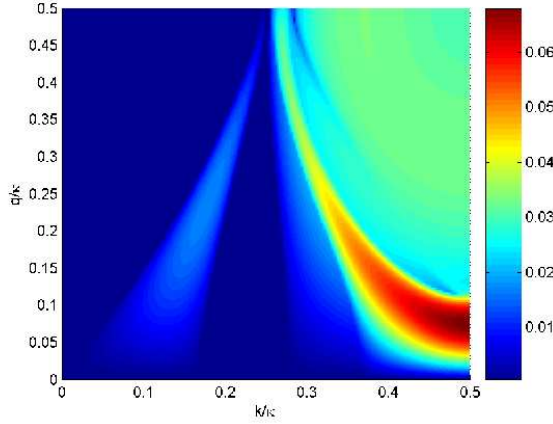

FIG. 5: Instability $\theta(q)$ of a Rb-Na condensate as a function of k and q for $v = 0.6085E_R$ (Colour online).

wavevector, q, the instability $\theta(q)$. As can be seen, this map is qualitatively different to that of a single component system. The map has two regions, small k and larger k. The large k behaviour is similar to the one component case in that instability sets in at $k \approx \kappa/4$ for modes with $q = \kappa/2$. At larger k the dominant (i.e. most rapidly growing) mode moves to longer wavelengths. Unlike the single component case, the short wavelength modes do not become stable as k increases and at $k = \kappa/2$ all q's are unstable. The small k regime is quite unlike the single component systems, there are long wavelength unstable modes even at $k = 0$ which persist up to a maximum k, with the dominant fluctuations moving

towards shorter wavelengths. This leaves a narrow window of Bloch wave vectors for which the system is stable.

The origin of the instability at small k lies in the fact that this system is unstable even in the absence of an optical lattice exhibiting a strong tendency to phase separate into single component domains. As shown by [8, 9] the condition for the mode with wavevector q to be stable in the absence of a lattice is

$$4q^4 + 2q^2 n \left(g_{11} + g_{22} \right) + n^2 \left(g_{11} g_{22} - g_{12}^2 \right) > 0 \tag{39}$$

so that if $g_{11} g_{22} < g_{12}^2$ only modes with sufficiently large q are dynamically stable. It is clear that the parameters for the Na-Rb mixture do not satisfy this stability criterion.

VI. USING AN OPTICAL LATTICE TO STABILIZE TWO-COMPONENT CONDENSATES

The depth of the lattice potential used above was chosen rather arbitrarily. We expect that increasing the depth of the optical lattice should enhance the stability of the NaRb system at low k because it confines the two components in different places. In particular, a very large value of V_0 should lead to an array of pure phase domains with the same periodicity as the optical lattice. In order to see how deep an optical lattice is required to stabilize the system we have carried out the stability analysis for the $k = 0$ Bloch states for a range of values of v for the NaRb mixture. Figure 6 shows a contour plot of the instability $\theta(q)$ as a function of V_0 and the fluctuation wave-vector q. As can be seen the instability is indeed suppressed as v increases. In figure 7 we show a contour map of the instability $\theta(q)$ as a function of k and q for $V_0 = 1.217 E_R$ which shows that although the $k = 0$ Bloch state has been stabilized, the instability re-appears at finite k - a deeper optical lattice is required to stabilize a moving condensate. Figure 8 shows the instability $\theta(q)$ as a function of k and q for $V_0 = 2.434 E_R$. In this case the phase separation instability is fully suppressed. The price for this supression is that the modulational instability at large k is much worse, with the dominant instability moved to higher q but with all q modes in the lowest two fluctuation bands being unstable once $k > \kappa/4$. An alternative way of showing the same physics is to plot the stability boundary for $k = 0$ Bloch states as a function of q and $ng_{11} (= ng_{22})$ for fixed $ng_{12} = 0.5 E_R$ for a range of values of v as shown in figure 9. Increasing v shrinks the
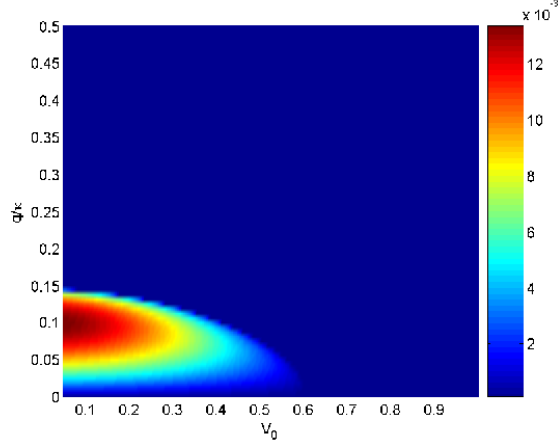
FIG. 6: A density map of the instability $\theta(q)$ for $k = 0$ as a function of fluctuation wave-vector q and optical lattice depth V_0 (colour online).
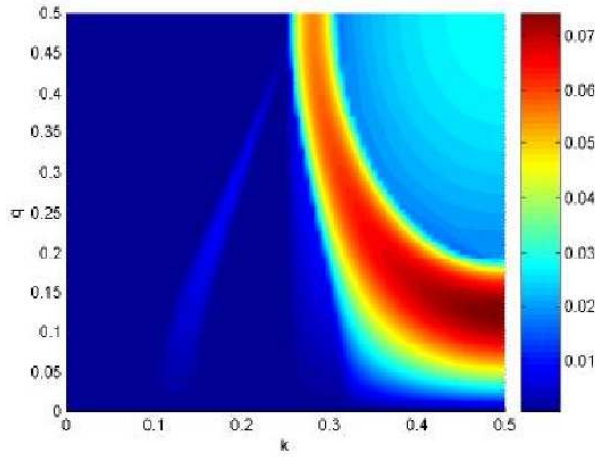

FIG. 7: Instability $\theta(q)$ of a Rb-Na condensate as a function of k and q for $V_0 = 1.217E_R$ (colour online).

region of instability below the line as one would expect.

Hence we have shown that two-component Bose condensates in 1d optical lattices can exhibit both the modulational instability at large Bloch wavevectors associated with single component systems and the instability to phase separation at small k that can occur in the absence of a lattice. Turning on the lattice enhances the latter instability but suppresses the former. Hence such optical lattices could be used to hold immiscible two-component systems in intimate contact and to move them around within a trap.
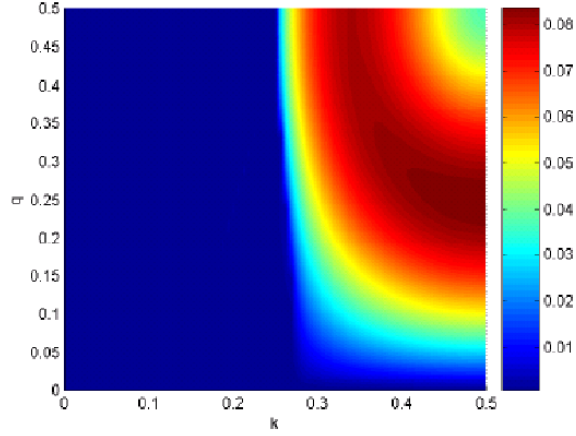
FIG. 8: Instability $\theta(q)$ of a Rb-Na condensate as a function of k and q for $V_0 = 2.434 E_R$ (colour online).
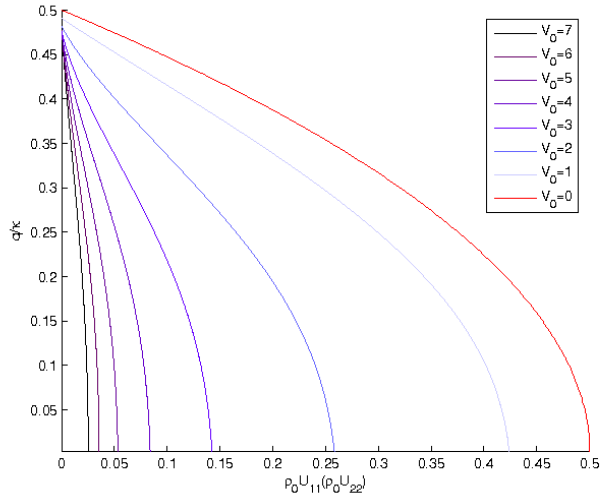

FIG. 9: The stability limit as a function for the largest unstable mode at $k = 0$ for a condensate with fixed $ng_{12} = 0.5 E_R$ as a function of $ng_{11} = ng_{22}$ for values of V_0 between 0 and $7 E_R$ (colour online).

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